ABSTRACT

The invention relates to the use of ratios, products and non-linear functions of adsorption, emission or scattering of light as variables in standard regression and chemometric techniques to predict a characteristic or property of a solid or liquid. The use of one or more non-linear functions within a relationship between measured spectral properties and characteristic properties of solutions and solids provides an improved means to determine a property when the intensities represent or relate to components that are colinear or interelated due to restraints associated with composition, chemical processes, or molecular structure. The invention relates to the use of ratios of Raman peak intensities to predict the properties of a solution or a solid such as pulp that is processed with the solution. The intensity of the Raman shifted light is used to create Raman peak intensity ratios. These Raman intensities are related to the concentration of species dissolved in the liquid. The Raman spectra are baseline corrected and the scattering from a water reference is subtracted before extraction of intensities for Raman peak intensity ratios. The Raman scattering intensities provide a good measure of the concentration of small, oxygenated molecules. The potential of an oxidative reductive process is conveniently determined using Raman peak intensity ratios. Relevant small molecules and complex ions in the pulp and paper industry include SO_4^{2-}, SO_3^{2-}, H_2O_2, ClO2, $HClO_3$, silicates, acetic acid, $HClO_3$, Chlorate ClO_3^-, Chlorous Acid $HClO_2$, Chlorite ClO_2^-, Hypochlorous Acid HClO. Hypochlorite ClO^-, phosphate, nitrate, nitrites. The method may also be used to determine a property related to the relative size, degree of polymerization, branching or network formation of complexing or polymerized species. The method may also be used to measure large molecules such as hemicellulose, extractives and pectic substances.